

***Ab initio* study of a monolayer ZrO₂ epitaxial on Si**

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Thin films of crystalline metal oxides grown on semiconductors have been of great scientific and technological interest because of their possible applications in electronic devices. One significant research aim is to achieve ferroelectricity in a crystalline and thin oxide film grown epitaxially on a semiconductor. This would be the key to realize non-volatile field-effect transistors in which the state of the system is retained by the oxide polarization. In this work, we study oxides that are not ferroelectric in the bulk but become ferroelectric as an ultrathin film on a semiconductor such as silicon. Thanks to the recent progress in epitaxial growth methods fabrication of such systems are also feasible.

In our study, we use density functional theory to first examine the interface of a single monolayer of ZrO₂ and Si. We show that a set of structures with a variety of positive and negative out-of-plane ferroelectric polarizations are stabilized. We present geometrical and electronic analyses of these structures. We also propose that a monolayer of ZrO₂ can be used as a buffer layer to induce ferroelectricity in thin perovskite oxides such as SrTiO₃ on Si which can couple the polarization of the oxide to the silicon carrier density. We analyze the layer-by-layer polarization profile of the Si-1ML ZrO₂-SrTiO₃ system and demonstrate that our proposal is viable. Finally we explore some aspects of switching between states of different polarization. We examine the transition barriers between metastable states using the nudged elastic bands method. We also analyze formation of differently polarized domains by mapping the system to an anisotropic Ising model with parameters determined by our *ab initio* theory.